

1. NUMERICAL DIFFERENTIATION

1.1. Problem statement. Assume that f is a known and sufficiently smooth function of x (the meaning of sufficiently smooth will be clear later). How can we find a numerical approximation to the derivative $f'(x)$ at a given point x_0 .

1.2. Test problems. In the class, three different test problems were suggested:

$$(1a) \quad f(x) = x^2, \quad x_0 = 0, \quad f'(x) = 2x$$

$$(1b) \quad f(x) = e^x, \quad x_0 = 10, \quad f'(x) = e^x$$

$$(1c) \quad f(x) = \sinh x, \quad x_0 = 1, f'(x) = \cosh x$$

In all cases, the exact solution is known, thus they are applicable for testing the algorithm, and the theoretical results which will be derived later.

1.3. Algorithm. Let us start with the definition of the derivative:

$$(2) \quad f'(x) = \lim_{h \rightarrow 0^+} \frac{f(x+h) - f(x)}{h}$$

which more or less automatically give us the simplest approximation to the derivative: For a given (small) $h > 0$, let

$$(3) \quad f'(x) \approx \hat{f}'(x_0) = \frac{f(x+h) - f(x)}{h}$$

where $\hat{f}'$ is the numerical approximation of f' .

1.4. Testing the algorithm. The next step is now to see if the algorithm (3) behaves reasonable. For each of the test problems an approximation to $f'(x_0)$ were computed, using two different values of h . In each case the absolute value of the error

$$(4) \quad e(h) = \hat{f}'(x_0) - f'(x_0)$$

were reported. The results are as follows:

$f(x)$	x_0	h	$\hat{f}'(x_0)$	$ e(h) $
x^2	0	0.01	0.01	0.01
		0.005	0.005	0.005
e^x	10	0.001	22037.48	11.0
			22031.97	5.51
$\sinh x$	1	0.1	1.5490	$5.90 \cdot 10^{-3}$
		0.05	1.5460	$2.94 \cdot 10^{-3}$

Remark 1.1.

- (1) The error $|e(h)|$ reduced by a factor 2 when the stepsize is reduced accordingly. Thus a reasonable hypothesis is:

$$e(h) \approx Ch, \quad \text{for some (unknown) constant } C.$$

This has to be proved, though.

- (2) In the second example, the error is 11 and 5.5 respectively, although h is smaller than in the other two examples. But the *relative* error $e(h)/f'(x_0)$ is $4.99 \cdot 10^{-3}$ and $2.50 \cdot 10^{-3}$, which is more reasonable.

1.5. Error analysis. The next step is an error analysis: What can we say about the error $e(h)$? In particular, do we have convergence, $e(h) \rightarrow 0$ when $h \rightarrow 0^+$?

In this case the error analysis is simply done by expressing the error as the difference between the numerical approximation and the exact solution, do a Taylor expansion of $f(x_0 + h)$ around x_0 , and then see which terms cancel out.

$$\begin{aligned} e(h) &= \frac{f(x_0 + h) - f(x_0)}{h} - f'(x_0) \\ &= \underbrace{\frac{f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(\xi) - f(x_0)}{h}}_{\text{Taylor expansion}} - f'(x_0) \\ &= \frac{1}{2}f''(\xi)h^2, \quad \xi \in (x_0, x_0 + h), \end{aligned}$$

Remark 1.2.

- (1) The value of $\xi \in (x_0, x_0 + h)$ is unknown. However, when h is small $f''(\xi) \approx f''(x_0)$.
- (2) The hypothesis $e(h) \approx Ch$ is correct with $C \approx f''(x_0)$ for sufficiently small values of h .
- (3) The theory above is only valid if f is twice continuously differentiable around x_0 .

1.6. Numerical verification of theoretical results, and a nice presentation of those. To verify the theoretical result, continue to measure the error $|e(h)|$ while different values of h , usually for stepsizes $h_0 \cdot 2^i$, $i = 1, 2, 3, \dots$, and make a log-log plot of the result. Choosing a log-log plot has two advantages: first, we can easily see the errors also for small values of h . But often, we want to verify that a numerical approximation of something has an error of order p , that is

$$|e(h)| \approx Ch^p \quad \Leftrightarrow \quad \log |e(h)| \approx p \log h + \log C,$$

and in a log-log plot the error as a function of h will appear as a straight line with slope p .

In Fig. [1](#) the result of such an experiment is presented. In this case $f(x) = \sinh x$, $x_0 = 1$ and $h_i = 2^i$, $i = 0, 1, \dots, 9$. Comparing with the reference line, we observe that the numerical order for h sufficiently small is 1. For large h , there is some deviation from the straight line. This is quite reasonable (why?).

The Python-code producing this figure is given in `numdiff1.py`. Try the other examples, and/or make your own.

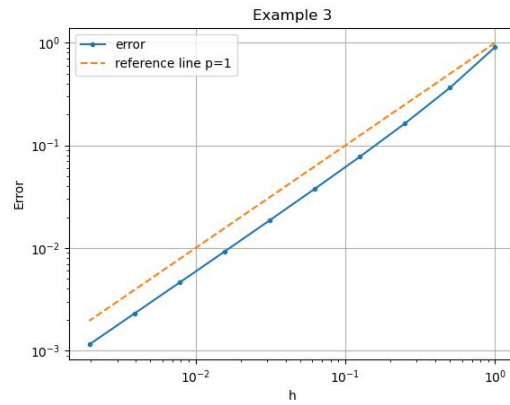


FIGURE 1. Error plot for example 3.

1.7. **What next?** Do we really have convergence, that is $e(h) \rightarrow 0$ for $h \rightarrow 0$. To check it, repeat the experiments for stepsizes $2^{-i}, i = 0, 1, 2, \dots, 50$. What do you observe now?

To be continued....

Email address: `anne.kvarno@ntnu.no`